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Editor's Choice

On the plastic driving force of grain boundary migration: A fully coupled phase field and crystal plasticity model

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ABSTRACT

Dislocations stored in heavily deformed materials play an important role in driving microstructure evolution. Here, we developed a full coupling model that concurrently couples the phase field method with crystal plasticity finite element analysis to study grain boundary (GB) migration under a plastic driving force. In our model, we describe multiple active grains in GB regions with crystal plasticity theory and use a weighted sum of their properties (i.e., stress and elastic/plastic potentials, etc.) to evaluate the plastic driving force for GB migration. The model can qualitatively capture the absorption of dislocations by mobile GBs through re-initialization of slip system resistances of newly active grains. A finite element based preconditioned Jacobian-free Newton-Krylov approach is used to simultaneously solve all the nonlinear partial differential equations for the coupled physics models. Determining model parameters and validation of the model are accomplished by simulating copper bicrystals and comparing the results to available experiments. This model provides a useful tool for effectively simulating GB migration in metals undergoing large plastic deformation. All the developments have been implemented in the MOOSE/MARMOT simulation package.

1. Introduction

Mechanical properties of polycrystalline alloys depend on the details of the microstructure, e.g., grain sizes and orientations, grain boundary (GB) networks, dislocation densities. Not only the grain size affects the mechanical properties of materials, but mechanical deformations can also alter the grain size. Both deformation-induced grain refinement [1–4] and grain coarsening [5,6] have been reported in experimental and computational studies. Therefore, understanding and predicting how GBs migrate in the presence of plastic deformation is important to the development of materials with optimized mechanical properties.

Computer simulations make it possible to track the evolution of stresses and strains as well as microstructural evolution *in operando* (i.e., during deformation) and they allow one to isolate different effects in the interplay between mechanical deformation and microstructural evolution. Therefore simulations provide a useful complementary approach to experiments.

Different modeling techniques have been used to study plastic deformation behaviors of materials. Atomistic simulations, such as those based on the molecular dynamics (MD) technique, are able to capture the effect of plastic deformation on GB migration and sliding [7,8]. However, this method cannot simulate microstructural changes in materials on typical experimental time scales. For instance, the deformation rate for standard MD simulations ($10^8 - 10^{10}$ s^{-1}) is much higher than in experiments ($10^{-3} - 10^{-4}$ s^{-1}). Modeling of deformation on typical experimental time scales is often accomplished by the use of finite element analysis, but in this method it can be challenging to efficiently track interface kinetics. A useful and highly versatile technique for modeling evolution of a microstructure, and more generally of interfaces, is the phase field method. This method can be coupled with a model of plastic deformation in order to simulate the effect of plastic behavior on microstructural evolution. A few approaches towards this goal have been reported so far, and they are summarized below.

A two-step coupling approach, proposed by Takaki et al. [9,10], Güvenç et al. [11] and Vondrous et al. [12], describes the deformation process and microstructural evolution with separate models that are coupled sequentially. This approach has been used to model static recrystallization process during annealing, where the stored energy of deformation is the main driving force for microstructural evolution. Specifically, the deformation prior to annealing is simulated by the finite element method (FEM) based

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on crystal plasticity theory. Subsequently, the deformed structure is mapped onto the phase field mesh as input, so that the stored deformation energy can be used to drive the evolution of the microstructure. The two-step method is relatively easy to implement, but the one-way data transfer reduces the accuracy of the results and such approach is not capable of modeling dynamic recrystallization, where the GB migration and plasticity mutually affect each other.

Abrivard et al. [13] developed an iteratively-coupled model which accounts for both the GB driving force due to the stored deformation energy and the dislocation absorption by mobile GBs. In their framework, the data is mutually exchanged at each time step between phase field and crystal plasticity models. This model is therefore more applicable to studies of phenomena such as dynamic recrystallizations [13,14]. While the model has many advantages, one of its limitations is that the coupling is hierarchical in nature due to the fact that the two individual physics models (i.e., mechanics/plasticity and phase field) are still solved separately and data exchange occurs only once per time step. This kind of loose coupling leaves open questions of stability and accuracy of the solutions, as discussed in Refs. [15,16]. In addition, the authors followed the grain growth model proposed by Kobayashi, Warren and Craig Carter [17,18] (often referred to as KWC model) which uses a single variable to describe the crystal orientations of all grains. This treatment of grain orientations can only deal with two dimensional problems. For three dimensional cases, an entirely different approach must be taken, for example using the quaternion representation [19]. In such case one would need to develop a completely different approach for coupling with the crystal plasticity model from what was done in Ref. [13].

One integrated approach taken by several authors involves incorporating dislocation dynamics into phase field using the microelasticity theory [20–22]. In this framework, both short-range and long-range interactions between dislocations are taken into account and the model can account for strain hardening. In the presence of interfaces such as GBs, geometrically necessary dislocations are often taken into account in the model to physically represent the effect of interfaces on the non-uniform plastic deformation [23]. This approach provides a high level of physical fidelity. However, the fine mesh resolution required to resolve dislocations makes this approach computationally prohibitive for simulating large-scale problems, especially when one wants to combine simulations of microstructural evolution with models of dynamic mechanical contacts as we intend to do in the future.

Another approach has been introduced by Gaubert et al. [24] and Cottura et al. [25]. These authors developed phase field models that incorporate phenomenological viscoplasticity and used these models to study rafting in Ni-base superalloys. These approaches are able to address the dynamic coupling between microstructural evolution and viscoplastic deformation. By adding strain gradient plasticity formalism into their model, Cottura et al. [25] were also able to study the effects of precipitate size on viscoplastic behavior. However, the above framework only considers coherent interfaces, and therefore it cannot be used to simulate GB migration. In addition, although there is a free energy term in the model associated with hardening, the corresponding parameters are deliberately chosen so that the plastic driving force vanishes. Consequently, plasticity evolves the microstructure only indirectly by decreasing the elastic stress due to plastic strain. In other words, only the elastic driving force on the interface migration is present. This kind of model that neglects the plastic driving force (or more precisely, that includes the impact of plasticity effect indirectly as described above) will be referred to as a weakly coupled model in this paper.

Here, we develop a multi-physics model that is coupled fully (i.e., partial differential equations (PDEs) for individual physics models are solved simultaneously) and strongly (i.e., we include plastic driving force on GB migration directly). In particular, we use crystal plasticity finite element (CPFE) method [23,26] to simulate the plastic deformation and phase field grain growth model [27] to effectively simulate the GB migration. We combine the FEM and Jacobian-free Newton-Krylov (JFNK) technique [28] to simultaneously solve the PDEs for both physics models (i.e., mechanics/plasticity and phase field) at each time step. More details of such FEM-JFNK approach will be discussed in Section 2.5. The theoretical framework developed in this paper has been implemented in the MOOSE/MARMOT simulation software [29,30] which was used to carry out all the simulations. Our model makes it possible to simulate the GB migration driven by plastic deformation. For instance, the model can be used to effectively model irregular grain growth in highly deformed materials. Note that the aim of our studies is to investigate GB migration within a bulk material and we do not include the effect of free surfaces as has been done by the authors of Refs. [31,32].

The remainder of this paper is organized as follows. In Section 2, we introduce the general framework of the coupling model and the strategy for solving systems of coupled PDEs that represent the two physics models in our study. In Section 3, we discuss the model parameters, including GB properties, and parameters for crystal plasticity model and the plastic potential. In Section 4, we apply the model to simulate compressive deformation of a Cu bicrystal to demonstrate the effect of plasticity on GB migration and to compare our results to published experiments where data is available. Finally a brief discussion and concluding remarks can be found in Section 5.

2. Methods

2.1. Phase field

The phase field method is a well established technique for simulating interface kinetics at the mesoscale, and it has been widely used for modeling solidification [33,34], solid-state phase transformation [35,36], grain growth [27], etc. In the phase field method, microstructure is represented numerically with a set of so-called phase field variables, which change continuously in space across the diffuse interfaces. The interfacial kinetics is modeled by evolving the phase field variables temporally according to a set of PDEs, which are the Cahn-Hilliard equation [37] for conserved variables and the Allen-Cahn equation [38] for non-conserved variables.

In this study we apply the grain growth model proposed by Chen [27]. In this model, each grain is represented using one of the order parameters $\{\eta_i\}$, which takes on the value of 1 within grains they represent, and change gradually to 0 elsewhere. According to the diffuse interface theory [39], the total system free energy can be written as

$$F = \int_V \left[f_0(\eta_1, \eta_2, \ldots, \eta_p) + \sum_i^p \frac{\kappa_i}{2} (\nabla \eta_i)^2 + \psi \right] \mathrm{d}V, \tag{1}$$

where V is the system's volume, $f_0(\eta_1, \eta_2, \ldots, \eta_p)$ is the bulk chemical free energy density, κ_i is the gradient energy coefficient. ψ is the stored deformation energy, which includes both elastic and plastic potential energies. These energy terms will be described in detail in Section 2.3. Following the proposal by Moelans et al. [40], we choose the chemical free energy density $f_0(\eta_1, \eta_2, \ldots, \eta_p)$ to be represented by a polynomial

$$f_0(\eta_1, \eta_2, \ldots, \eta_p) = \mu \left[\sum_{i=1}^{p} \left(-\frac{1}{2}\eta_i^2 + \frac{1}{4}\eta_i^4 \right) + \gamma \sum_{i=1}^{p} \sum_{j \neq i} \eta_i^2 \cdot \eta_j^2 + \frac{1}{4} \right], \tag{2}$$